

PREDICTION OF A MULTIVARIATE SPATIAL RANDOM FIELD WITH CONTINUOUS, COUNT AND ORDINAL OUTCOMES

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ABSTRACT

As most georeferenced data sets are multivariate and concern variables of different kinds, spatial mapping methods must be able to deal with such data. The main difficulties are the prediction of non-Gaussian variables and the dependence modelling between processes. The aim of this paper is to present a new approach that permits simultaneous modelling of Gaussian, count and ordinal spatial processes. We consider a hierarchical model implemented within a Bayesian framework. The method used for Gaussian and count variables is based on the generalized linear model. Ordinal variable is taken into account through a generalization of the ordinal probit model. We use the moving average approach of Ver Hoef and Barry to model the dependencies between the processes.

INTRODUCTION

The prediction of multivariate spatial processes from collected data is a major issue in many research areas including biological sciences (McBratney et al., 2000), epidemiology (Golam Kibria et al., 2002) and economics (Chica-Olmo, 2007; Gelfand et al., 2007). In most cases few data are available as they are expensive to collect. Moreover, available data are often of different nature. For example, in geological studies, concentrations of elements (continuous variable), granularity (ordinal variable) and coloration (nominal variable) are classically measured for soil characterization (Epron et al., 2006). Spatial mapping methods thus have to be able to handle related data of different nature. This raises two difficulties: the prediction of multivariate discrete random fields and the modelling of the dependence between continuous and discrete spatial processes.

In the univariate case, the prediction of continuous spatial processes has been widely studied and implemented (Cressie, 1991; Wackernagel, 2003). For discrete random fields, methods based on geostatistics and point processes have been developed: disjunctive kriging (Webster and Oliver, 1990), truncated Gaussian random fields (Chilès and Delfiner, 1999), object models and Markov random fields (Molchanov, 1997; Cressie, 1991). New models have been defined, particularly to deal with count variables. Diggle et al. (1998) proposed to embed linear kriging methodology within the framework of the generalized linear mixed model where the random effect is modelled by a Gaussian spatial process. Diggle et al. (1998) proposed to model count data with a Poisson distribution whose intensity is the unobserved value of a random measure. They modelled the random intensity using a gamma process. Such models are now often described in the hierarchical Bayesian framework (Banerjee et al., 2004).

The prediction of multivariate spatial processes has been widely studied in the last few decades (Cressie, 1991; Wackernagel, 2003). The proposed models are efficient but they require certain restricting assumptions: normality for linear cokriging methods (Cressie, 1991) or isofactorial model assumption for disjunctive cokriging (Rivoirard, 1991; Chilès and Delfiner, 1999). Modelling the dependence between variables is closely linked to the prediction method chosen. Cokriging methods are based on a full covariance structure model whereas disjunctive cokriging methods involve hypotheses based on bivariate distributions. In the latter, the determination of the bivariate distributions can be tedious and the classical isofactorial Gaussian model may be unsuitable. In this paper we propose an approach based on a full covariance structure model. Many studies have been published on this topic. The intrinsic correlation model is the simplest multivariate covariance model (Wackernagel, 2003). A generalization, the coregionalization model, enables the multivariate correlation structure to be taken into account at different scales of a phenomenon (Grzebyk and Wackernagel, 1994; Banerjee et al., 2004). The latter class of covariance models assumes that the correlation structures for and between each variable are the same up to a constant. Moreover, the choice of each elementary covariance structure in coregionalization models should ensure that the global covariance matrix is positive definite. The use of these approaches is strongly restricted by these two constraints. Barry and Ver Hoef (1996) defined a new family of valid variograms using moving average functions. Ver Hoef and Barry (1998) generalized their approach to the multivariate Gaussian case by defining cross pseudo variograms. They built dependent Gaussian processes by convolving white noise process with a moving average function (Higdon, 2001; Calder and Cressie, 2007). The moving average constructions are attractive because the obtained variograms are very flexible. Although many studies have been concerned with multivariate predictions the problems raised by variables of different nature are no nearer solutions.

The aim of this paper is to propose a new unified approach that permits simultaneous modelling of Gaussian, count and ordinal spatial processes and to apply this method to simulated data set. In section 2, we present the spatial

hierarchical model. A simulation study is presented in section 3 and results are discussed. Finally, in section 4, we draw some conclusions and give some perspectives for future work.

METHODS: HIERARCHICAL SPATIAL MODEL

Model

The model is specifically designed to take into account variables of different kinds. Before describing the model, let's first define some notations.

Let (s_1, \dots, s_N) be the sampled locations. Let $Y_1(s_i)$ (resp. $Y_2(s_i)$, $Y_3(s_i)$) be a Gaussian variable (resp. a Poisson variable, an ordinal variable with J modalities) at location s_i . Let $Y_k(\mathbf{s}) = (Y_k(s_1), \dots, Y_k(s_N))$, $k = 1, 2, 3$, be the vector of the variable Y_k observed at all locations. Let $\mathcal{N}_d(\mathbf{m}, \Sigma)$ be the d -dimensional multivariate normal distribution with mean vector \mathbf{m} and covariance matrix Σ , and $\mathcal{P}(\lambda)$ be the Poisson distribution with parameter λ .

The spatial model is based on a hierarchical framework like Wolpert and Ickstadt's one (?). This approach accommodates complexity in high-dimension models by decomposing a model into a series of simpler conditional levels. The Gaussian variable $Y_1(s)$ as well as the Poisson variable $Y_2(s)$ depend on latent variables $\beta_1(s)$ and $\beta_2(s)$ respectively. Conditionnally to $\beta_1(s)$ and $\beta_2(s)$, the variables $Y_1(s)$ and $Y_2(s)$ are independent. For the Gaussian and Poisson variables, we follow the generalized linear model proposed by Diggle et al. (1998):

$$Y_1(s_i) | \mu_1, \beta_1(s_i), v_1 \sim \mathcal{N}(\mu_1 + \beta_1(s_i), v_1^2), \quad (1)$$

$$Y_2(s_i) | \mu_2, \beta_2(s_i) \sim \mathcal{P}(\exp(\mu_2 + \beta_2(s_i))). \quad (2)$$

To model the ordinal variable, we have to introduce two nested latent levels: (i) the first one allows to define the multivariate ordinal probit model as proposed by Chib and Greenberg (1998), (ii) the second one allows to generalize the multivariate ordinal probit model to the spatial case. Then the ordinal variable $Y_3(s)$ is modeled through equations (3) and (4):

$$\mathbb{P}(Y_3(s_i) = j | Z_3(s_i), \alpha_3, \beta_3(s_i), \mu_3) = \mathbb{P}(Z_3(s_i) \in]\alpha_{3;j-1}, \alpha_{3;j}] | \beta_3(s_i), \mu_3), \quad (3)$$

$$Z_3(s_i) | \beta_3(s_i), \mu_3 \sim \mathcal{N}(\mu_3 + \beta_3(s_i), 1) \quad (4)$$

where $\alpha_3 = (\alpha_{3;0}, \alpha_{3;1}, \dots, \alpha_{3;J})$ denote the vector of thresholds related to the Gaussian variable Z_3 . By convention, $\alpha_{3;0} = -\infty$ and $\alpha_{3;J} = +\infty$. Expressions (1), (2), (3) and (4) make the first level of the hierarchical model. This approach can be generalized to K_1 Gaussian variables, K_2 Poisson variables and K_3 ordinal variables.

The spatial dependency between the processes $Y_k(\cdot)$ is carried by the latent Gaussian processes $\beta_k(\cdot)$, $k = 1, \dots, 3$. The processes are built according to the moving average construction proposed by Ver Hoef and Barry (1998), that is to say by convolving a moving average function with a mixture of white noise processes.

Let f_k , $k = 1, 2, 3$ be a moving average function defined on \mathbb{R}^2 . θ_k denotes the vector of parameters of f_k . Let T_k , $k = 1, 2, 3$ be a linear combination of white noise processes:

$$T_k(x|\rho_k, \Delta_k) = \sqrt{1 - \rho_k^2} W_k(x) + \rho_k W_0(x - \Delta_k)$$

where $W_k(\cdot)$, $k = 0, 1, 2, 3$ is a white noise process and ρ_k , $k = 1, 2, 3$ belongs to the interval $[-1, 1]$. The variable $\beta_k(s_i)$ is defined by:

$$\beta_k(s_i) = \int_{\mathbb{R}^2} f_k(x - s_i|\theta_k) T_k(x|\rho_k, \Delta_k) dx$$

with $\Delta_k = (\Delta_{k,x}, \Delta_{k,y}) \in \mathbb{R}^2$.

So the conditional distribution of $\beta(\mathbf{s}) = (\beta_1(\mathbf{s}), \beta_2(\mathbf{s}), \beta_3(\mathbf{s}))$ is a Gaussian distribution with zero mean and covariance matrix \mathbf{C} :

$$\beta(\mathbf{s})|\theta_1, \theta_2, \theta_3 \sim \mathcal{N}_{3N}(\mathbf{0}, \mathbf{C}).$$

This makes the second level of the hierarchy. One advantage of this construction is that the expression of the covariance matrix \mathbf{C} is known:

$$C_{kk}(\mathbf{h}) = \text{Cov}[\beta_k(\mathbf{s}), \beta_k(\mathbf{s} + \mathbf{h})] = \int_{\mathbb{R}^2} f_k(\mathbf{x}) f_k(\mathbf{x} - \mathbf{h}) d\mathbf{x}, \quad (5)$$

$$C_{km}(\mathbf{h}) = \text{Cov}[\beta_k(\mathbf{s}), \beta_m(\mathbf{s} + \mathbf{h})] = \rho_k \rho_m \int_{\mathbb{R}^2} f_k(\mathbf{x}) f_m(\mathbf{x} - \mathbf{h} + \Delta_m - \Delta_k) d\mathbf{x}. \quad (6)$$

$\rho_{km} \equiv \rho_k \rho_m$ is the crosscorrelation between white noise processes T_k , T_m and $\Delta = (\Delta_k, \Delta_m)$ expresses the shift-asymmetry of cross spatial dependance (Barry and Ver Hoef, 1996). Depending on the choice of the moving average functions, the calculation of the integral is either explicit or complex. In the latter case, each element of the matrix can be seen as an autocorrelation in signal theory and can be calculated with the Fast Fourier Transform (Ver Hoef et al., 2004).

The third level of the hierarchical model consists in giving the *prior* distributions on the parameters. The *prior* on μ_1, μ_2, μ_3 is an uniform distribution. For v_1^2 , we chose to use an inverse gamma conjugate *prior* specification $v_1^2 \sim IG(a, b)$ where a et b are fixed. We assign an independent uniform *prior* to each spatial dependence parameter $\theta_i, i = 1, 2, 3$, $\rho = (\rho_1, \rho_2, \rho_3)$ and $\Delta = (\Delta_1, \Delta_2, \Delta_3)$. The *prior* distribution of the thresholds α_3 is the order distribution of $J - 2$ uniform random variables.

Inference

While the classical approach by maximum likelihood is difficult, the use of conditional independency and the introduction of the latent Gaussian variable Z_3 in the ordinal case allow the evaluation of the *posterior* distribution of the parameters. Using the *prior* distributions, the joint distribution is given by:

$$\begin{aligned}
& \pi(\mu_1, \mu_2, \mu_3, \beta(\mathbf{s}), Z_3(\mathbf{s}), v_1, \alpha, \theta_2, \theta_2, \theta_3 | Y(\mathbf{s})) \\
& \propto \exp \left\{ -\frac{1}{2v_1^2} (Y_1(\mathbf{s}) - \mu_1 - \beta_1(\mathbf{s}))(Y_1(\mathbf{s}) - \mu_1 - \beta_1(\mathbf{s})) \right\} \\
& \times \prod_{i=1}^N \left[\frac{[\exp(\mu_2 + \beta_2(s_i))]^{Y_2(s_i)} \exp\{\exp(\mu_2 + \beta_2(s_i))\}}{Y_2(s_i)!} \right] \\
& \times \prod_{i=1}^N \left[\exp \left\{ -\frac{1}{2} (Z_3(s_i) - \mu_3 - \beta_3(s_i))^2 \right\} \mathbb{1}(Z_3(s_i) \in [\alpha_{3;Y_3(s_i)-1}; \alpha_{3;Y_3(s_i)}]) \right] \\
& \times \exp \left\{ -\frac{1}{2} \beta(\mathbf{s}) C^{-1} \beta(\mathbf{s}) \right\} \pi(v_1^2)
\end{aligned}$$

where $\mathbb{1}$ denotes the indicator function.

The marginal posterior distributions for each of these parameters can be obtained through the implementation of a Markov chain Monte Carlo (MCMC) simulation scheme. Parameters $\mu_1, \mu_3, \beta_1(\mathbf{s}), \beta_3(\mathbf{s}), v_1, \alpha_3$ are drawn iteratively from their full conditional distributions :

$$\mu_1 | \dots \sim \mathcal{N} \left(\frac{1}{N} \sum_{i=1}^N (Y_1(s_i) - \beta_1(s_i)), \frac{v_1^2}{N} \right),$$

$$\mu_3 | \dots \sim \mathcal{N} \left(\frac{1}{N} \sum_{i=1}^N (Z_3(s_i) - \beta_3(s_i)), \frac{1}{N} \right),$$

$$v_1^2 | \dots \sim IG \left(a + \frac{N}{2}, b + \frac{\sum_{i=1}^N (Y_1(s_i) - \mu_1 - \beta_1(s_i))^2}{N} \right),$$

$$\begin{aligned}
& \alpha_{3;j} | \dots \sim \\
& \mathcal{U} [\max(\max(Z_3(s_i) | Y_3(s_i) = j), \alpha_{3;j-1}); \min(\min(Z_3(s_i) | Y_3(s_i) = j+1), \alpha_{3;j+1})],
\end{aligned}$$

$$\beta_1(\mathbf{s}) | \dots \sim \mathcal{N}_N(m_1^*, V_1^*) \text{ with } \begin{cases} V_1^* = \left(V_1^{-1} + \frac{1}{v_1^2} I \right)^{-1} \\ m_1^* = V_1^* \left(V_1^{-1} m_1 + \frac{1}{v_1^2} (Y_1(s) - \mu_1) \right) \end{cases}$$

where m_1 and V_1 are respectively the conditional expectancy and the covariance matrix of $\beta_1(\mathbf{s})$ given $\beta_2(\mathbf{s})$ and $\beta_3(\mathbf{s})$,

$$\beta_3(\mathbf{s}) | \dots \sim \mathcal{N}_N(m_3^*, V_3^*) \text{ with } \begin{cases} V_3^* = (V_3^{-1} + I)^{-1} \\ m_3^* = V_3^* (V_3^{-1} m_3 + (Z_3(s) - \mu_3)) \end{cases}$$

where m_3 and V_3 are respectively the conditional expectancy and the covariance matrix of $\beta_3(\mathbf{s})$ given $\beta_1(\mathbf{s})$ and $\beta_2(\mathbf{s})$.

The vector $\beta_2(\mathbf{s})$ is updated by an adaptative version of a Metropolis Langevin algorithm (Atchade, 2006). Let $\pi(\beta_2(\mathbf{s}))$ be the target distribution. The proposal

distribution is given by:

$$q_h(\beta_2^*(\mathbf{s})|\beta_2(\mathbf{s})) \sim \mathcal{N}\left(\beta_2(\mathbf{s}) + \frac{h^2}{2}D(\beta_2(\mathbf{s})), h^2I\right)$$

where

$$D(\beta_2(\mathbf{s})) = \frac{\delta}{\max(\delta, |\nabla \ln(\pi(\beta_2(\mathbf{s})))|)} \nabla \ln(\pi(\beta_2(\mathbf{s}))).$$

∇ is the gradient operator, $\delta > 0$ is a fixed constant and $h > 0$ is a scale parameter. The proposed value $\beta_2^*(\mathbf{s})$ is accepted with probability

$$\min\left(1, \frac{\pi(\beta_2^*(\mathbf{s}))q_h(\beta_2(\mathbf{s})|\beta_2^*(\mathbf{s}))}{\pi(\beta_2(\mathbf{s}))q_h(\beta_2^*(\mathbf{s})|\beta_2(\mathbf{s}))}\right).$$

The scale parameter h is updated at each iteration of the algorithm in order to obtain a acceptance rate of 0,574.

The spatial dependence parameters $\theta_i, i = 1, 2, 3$, ρ and Δ are sampled from a Metropolis step (Hastings, 1970). Each vector θ_i , each term of ρ and each vector Δ_k is updated separately. The proposal distribution of each parameter is a normal distribution centered on the current value of the parameter. If there are constraints on the parameter, the value is proposed according to a truncated normal distribution.

In the bivariate case, we can notice that the parameters ρ_k and ρ_m are not identifiable; only the product $\rho_{km} = \rho_k \rho_m$ can be identify. To ensure that all parameters are identifiable, the threshold $\alpha_{3,1}$ related to the ordinal variable is fixed to 0 (Cowles, 1996). Initial values of the parameters for the MCMC inference are randomly chosen. But it is better to run the algorithm in the univariate case for each variable and to take the obtained estimations as initial values for the multivariate procedure.

RESULTS AND DISCUSSION

The model is applied on simulated data sets. We simulated bivariate spatial data of various nature using moving average functions. 250 spatial locations were randomly chosen on $[-10; 10] \times [-10; 10]$. At each location s , we simulated two dependent variables $Y_{k_1}(s)$ and $Y_{k_2}(s)$. Following the previous notations, $k_1 = k_2 = 1$ corresponds to the bivariate Gaussian case while $k_1 = 2$ and $k_2 = 3$ corresponds to the Poisson-Ordinal case. No asymmetry-shift was introduced, so $\Delta_k = (0, 0)$, $k = k_1, k_2$. The chosen moving average functions had a Gaussian form: $f_k(x, y) = \sigma_k \exp\left(-\frac{(x^2 + y^2)}{\phi_k}\right)$, $k = k_1, k_2$ and the simulated ordinal variables had 3 modalities. We focus on the estimation of the five parameters σ_{k_1} , ϕ_{k_1} , σ_{k_2} , ϕ_{k_2} and $\rho_{k_1 k_2}$. The estimations are the posterior means of the distribution sampled from the MCMC scheme. The standard deviation of the distribution is given in brackets. Results are presented in Table .

The estimates of the parameters are consistent with the values used for simulations. For Gaussian and Poisson variables, parameters are well estimated. These results

Table 1: Parameters estimation from simulated data sets. For each data set, true values of parameters are given on first line and estimates on the second line. The standard deviation are given in brackets. $k_i = 1$ (resp. $k_i = 2$, $k_i = 3$), $i = 1, 2$ denotes Gaussian (resp. Poisson, ordinal) variables.

	σ_{k_1}	ϕ_{k_1}	σ_{k_2}	ϕ_{k_2}	$\rho_{k_1 k_2}$
$k_1 = 1$	10	2	20	4	0.5
$k_2 = 1$	10.69 (0.59)	2.02 (0.07)	19.80 (1.37)	3.75 (0.17)	0.54 (0.06)
$k_1 = 1$	10	2	1	0.2	0.5
$k_2 = 2$	9.38 (0.53)	1.88 (0.10)	0.96 (0.28)	0.16 (0.07)	0.71 (0.17)
$k_1 = 1$	10	2	20	4	0.5
$k_2 = 3$	9.02 (0.49)	1.83 (0.08)	18.69 (2.32)	3.18 (0.36)	0.42 (0.08)
$k_1 = 2$	1	0.2	0.5	2	0.3
$k_2 = 2$	1.55 (0.21)	0.14 (0.03)	0.41 (0.03)	1.82 (0.17)	0.18 (0.12)
$k_1 = 2$	0.5	2	2	4	0.5
$k_2 = 3$	0.51 (0.03)	2.44 (0.16)	2.05 (0.43)	3.24 (0.64)	0.47 (0.11)
$k_1 = 3$	1	3	2	3	0.5
$k_2 = 3$	0.85 (0.16)	2.47 (0.47)	1.40 (0.28)	3.09 (0.69)	0.44 (0.12)

remain true even if the number of observations is low. The convergence speed is high. On the contrary, parameter estimation for ordinal variables requires more iterations to obtain the convergence of the chain (Figure 1). In fact, the burn-in duration is longer due to two levels of latent variables (Z_3 and $\beta_3(\mathbf{s})$). The thresholds related to the underlying Gaussian variable Z are particularly difficult to estimate and their variances are often high. For the Gaussian-Ordinal data set, the estimate of the threshold $\alpha_{3,2}$ is equal to 29.27 while the true value of the parameter is equal to 35.95. Its standard deviation is around 2.8. The thresholds related to the Poisson-ordinal data set and the ordinal-ordinal data set are better estimated. The absolute deviations between the estimates and the true values are less than 0.79 and the standard deviations of the estimates vary between 0.18 and 0.6. In our algorithm, these thresholds are updated by Gibbs sampling. An alternative could be to update α_3 by a Metropolis step as proposed by Cowles (1996) in order to improve the convergence of the chain. The correlation ρ between variables is well estimated for any pair of variables except in the case of Gaussian and Poisson variables where ρ is always over estimated. Here spatial locations were randomly chosen. Simulations have shown that if the spatial locations are aggregated, the accuracy of the estimations decreases.

It is possible to simulate and estimate parameters for more than 2 variables. But the inference procedure could become computationally intensive and time consuming because of the size of handled covariance matrix in this case.

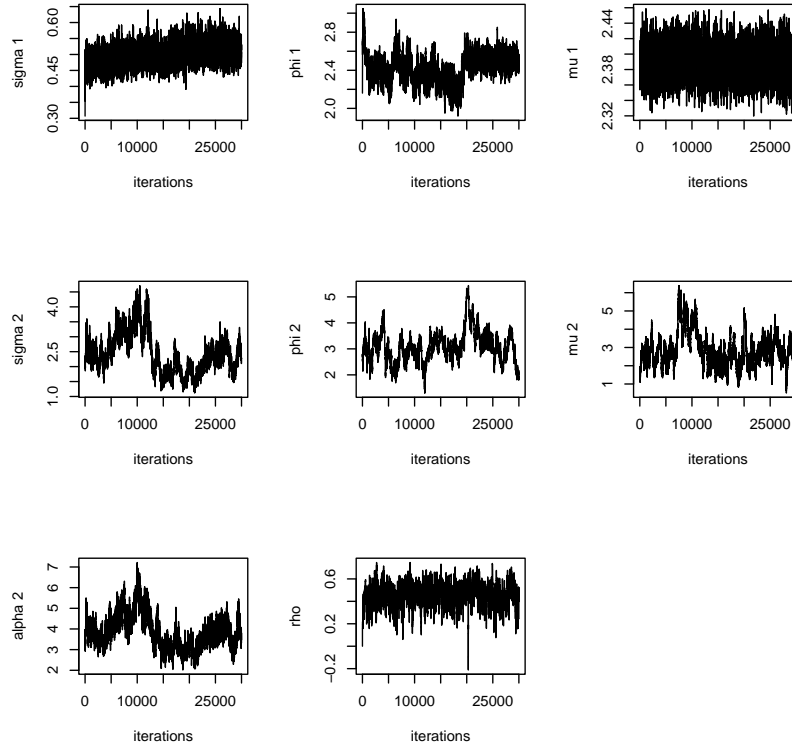


Figure 1: Sampling from full conditional distributions in the Poisson-Ordinal case

The choice of the moving average function can be questioned. The chosen form f_k is particularly pleasant because of the little number of parameters and the simple evaluation of the integrals in equations (5) and (6). More flexible functions could be used like exponential kernel, disk-based kernel (Kern, 2000) if the number of parameters is reasonable.

CONCLUSION

The proposed approach permits modelling a spatial multivariate random field made of variables of different nature. A unified methodology (generalized linear model) can be applied for Gaussian, Poisson and ordinal variables through the introduction of Gaussian latent variable in the discrete case. Although the estimation procedure is time consuming, this approach is an interesting alternative to disjunctive cokriging for the prediction of ordinal variables. The modelling of the dependence between the processes by the moving average approach has the advantage to be

very flexible. Anisotropic data can be dealt with if a convenient moving average function is chosen. An extension of the model can be considered for nominal variable. In the same way we have generalized the ordinal probit model to deal with ordinal variable, we can generalize the multinomial probit model to take into account nominal variables.

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